Verification and Validation in Computational Engineering and Sciences

Serge Prudhomme

Département de mathématiques et de génie industriel
Ecole Polytechnique de Montréal, Canada

SRI Center for Uncertainty Quantification
King Abdullah University of Science and Technology, Saudi Arabia

TERATEC 2015 FORUM
Ecole Polytechnique, Palaiseau, France
June 23-24, 2015

POLYTECHNIQUE MONTRÉAL
LE GÉNIE EN PREMIÈRE CLASSE

KAUST

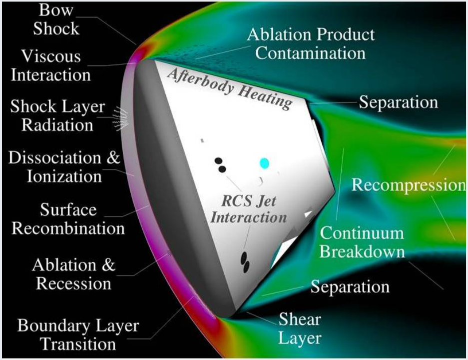
Outline

- Introduction and definitions.
- Description of validation process.
- Numerical examples.
  - Data model reduction
  - Model selection
- Concluding remarks

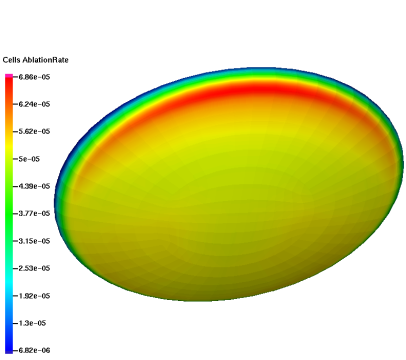
Model validation requires HPC!

Introduction

Vehicle during atmospheric entry

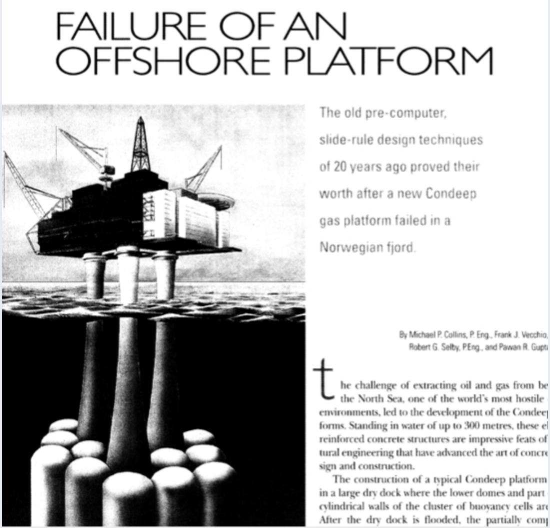


Ablation rate



Project conducted at PSAAP Center at ICES, UT Austin.
Objective: predict the ablation rate of a vehicle during atmospheric entry.

SLEIPNER A Offshore Plateform – Norway, 1991



FAILURE OF AN OFFSHORE PLATFORM

The old pre-computer, slide-rule design techniques of 20 years ago proved their worth after a new Condeep gas platform failed in a Norwegian fjord.

By Michael P. Collins, P. Eng., Frank J. Vecchio, Robert G. Selby, P.Eng., and Pawan R. Gupt

the challenge of extracting oil and gas from be the North Sea, one of the world's most hostile environments, led to the development of the Condee forms. Standing in water of up to 300 metres, these e reinforced concrete structures are impressive feats of tural engineering that have advanced the art of concre sign and construction.

The construction of a typical Condeep platform in a large dry dock where the lower domes and part cylindrical walls of the cluster of buoyancy cells ar After the dry dock is flooded, the partially com

- Dégâts: \$700 millions
- Analyse par Eléments Finis
- Logiciel Nastran
- Contraintes sous-estimées
- Structure tricell

Predictive Science: The Fundamentals

MATHEMATICAL MODEL:

A collection of mathematical constructions that represent the essential aspects of a system in a usable form (a mathematical representation of observations and theory proposed for explaining specific physical phenomena).

QUANTITIES OF INTEREST:

Specific objectives that can be expressed as the target outputs of a model (mathematically, they are often defined by functionals of the solutions and provide focus on the goal of scientific computation).

ABSTRACT MATHEMATICAL MODEL:

A mathematical model determines a map of physical parameters $\theta \in M$ into theoretical observables $Q \in \mathcal{D}$ for various scenarios $s \in \mathcal{S}$:

$$\text{Evaluate } Q(u(\theta, s)) \text{ s.t. } \quad \mathcal{A}(\theta, s; u) = 0, \quad \text{given } \theta \in M$$

with
$\mathcal{A} =$ The mathematical model
$\theta =$ The model (material) parameters
$s =$ The particular scenario on which the model is applied
$Q =$ The quantity of interest (observable) for scenario s

COMPUTATIONAL MODEL:

A discretization (or corruption) of a mathematical model designed to render it to a form that can be processed by computing devices.

$$\text{Evaluate } Q(u_h(\theta, s)) \text{ s.t. } \quad \mathcal{A}_h(\theta, s; u_h) = 0, \quad \text{given } \theta \in M$$

Verification

The process of determining the accuracy with which a computational model can produce results deliverable by the mathematical model on which it is based.

"Do we solve the equations right?" (Roache, 2009)

- Code Verification:
  - Manufactured solution method;
  - Estimation of rates of convergence; etc.
- Solution Verification:
  - It is based on a posteriori error estimation and adaptive methods (with respect to quantities of interest).
  - Its main objective is to verify that discretization parameters (in space, time, and stochastic dimension) and numerical parameters (model reduction method, nonlinear solver, etc.) are correctly chosen.

Validation

The process of determining the accuracy with which a model can predict observed physical events (or the important features of a physical reality).

”Do we solve the right equations?” (Roache 2009)

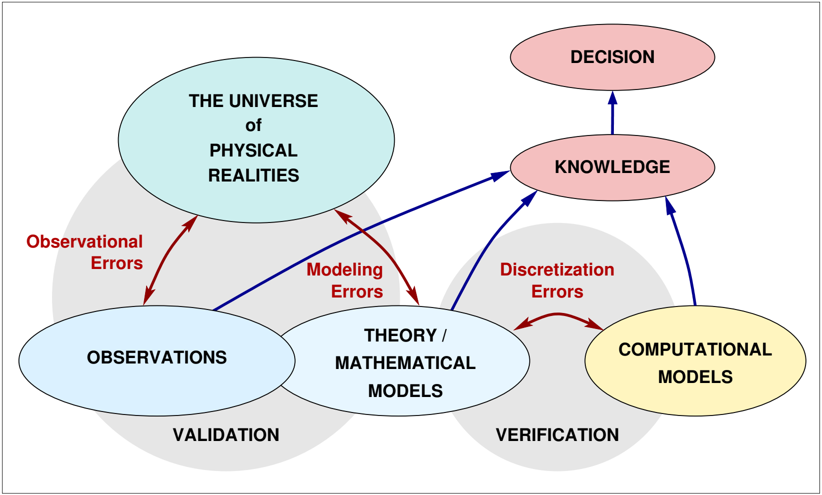
An art, not a science (yet) . . . It involves many a priori choices:

- Experiments or observations, splitting between calibration and validation datasets.
- Likelihood and prior in Bayesian inference.
- Acceptance metric to assess the validity of the model, etc.

An iterative process . . .

- Goal is to test as many hypotheses of the model as possible.

Paths to Knowledge



Oden and Prudhomme, IJNME (Sept. 2010)
Oden, Moser, and Ghattas, SIAM News, (Nov. 2010)

The Path of Truth . . .

"If error is corrected
whenever it is recognized as such,
the path to error
is the path of truth."

Hans Reichenbach (1891- 1953)
The Rise of Scientific Philosophy, 1951.

Control of Errors

Errors are all a matter of comparison!

- Code Verification: Using the method of “manufactured solutions”, for example, we can easily compare the computed solution with the manufactured solution.
- Solution Verification: In this case, the solution of the problem is unknown and one can use a posteriori error estimates to assess the accuracy of the approximate solutions.
- Calibration Process: Comparison of observable data with model estimates of the observables.
- Validation Process: The main idea behind validation is to know whether a model can be used for prediction purposes.

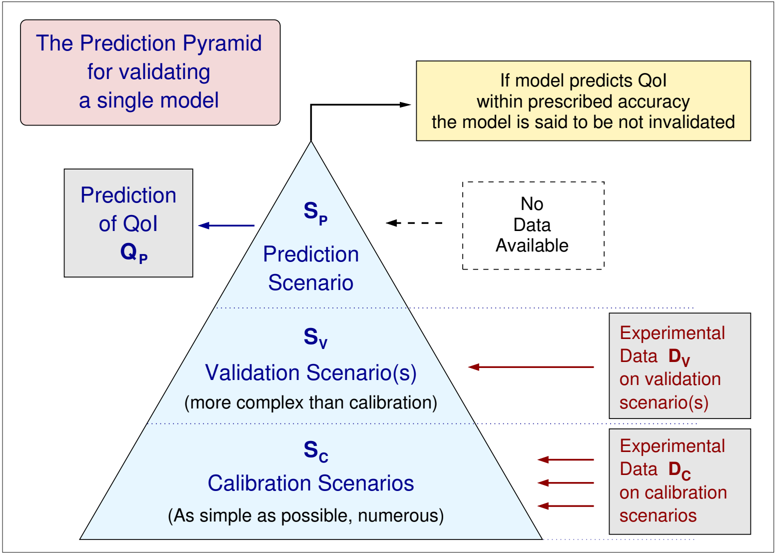
$\Rightarrow$ What should we compare in this case?

Model Validation

1. Is the model a good model? How good is the model? What is a good model?
2. Experimental data.
3. Calibration: Identification of model parameters in order that the model reproduce experimental measurements. Bayesian inference:

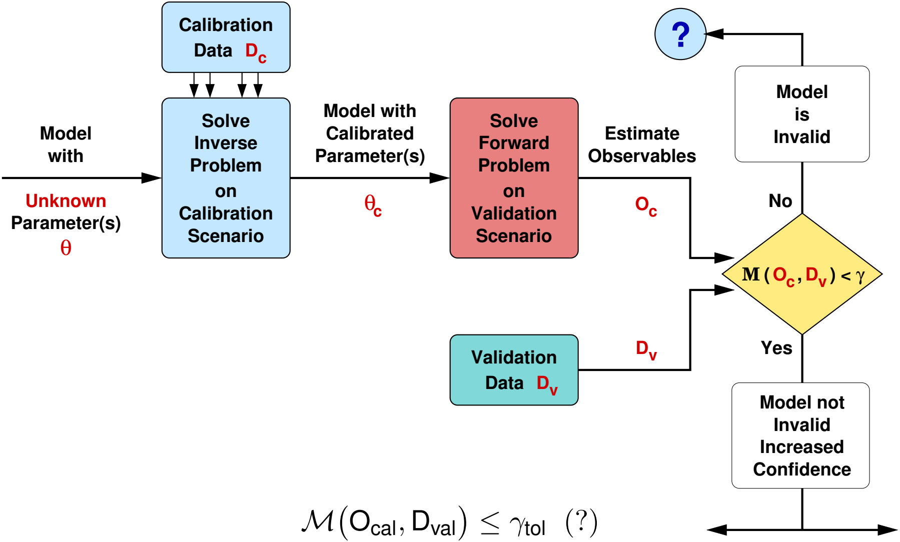
$$\boxed{p(\boldsymbol{\theta}|\boldsymbol{D}) = \frac{L(\boldsymbol{\theta}|\boldsymbol{D})\ p(\boldsymbol{\theta})}{p(\boldsymbol{D})}} \quad \text{where} \quad \begin{cases} \boldsymbol{D} \in \mathbb{R}^n & = \text{Calibration data} \\ L(\boldsymbol{\theta}|\boldsymbol{D}) & = \text{Likelihood} \\ p(\boldsymbol{\theta}) & = \text{Prior} \\ p(\boldsymbol{\theta}|\boldsymbol{D}) & = \text{Posterior} \end{cases}$$

4. Assessment with respect to a quantity of interest on a prediction scenario (cannot be measured or observed, otherwise it would not be a prediction any longer).
5. Definition of an acceptance metric.



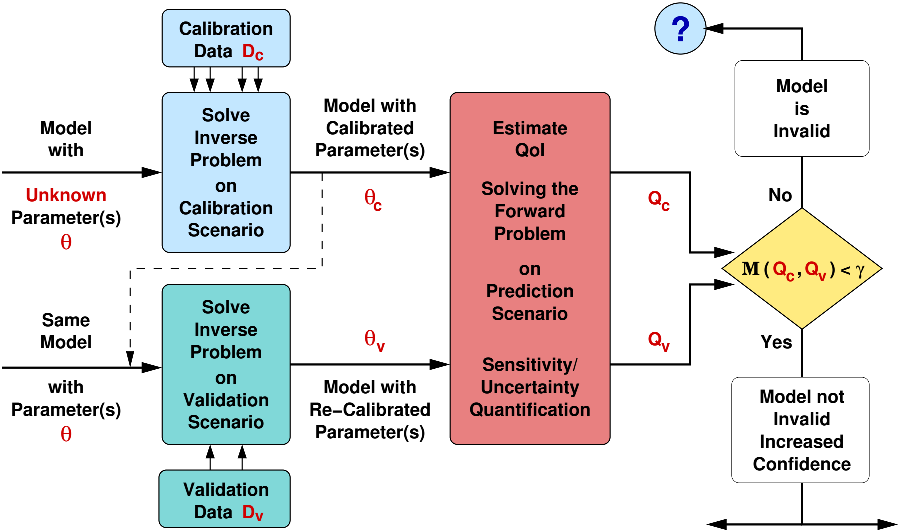
The Validation Pyramid

Classical Approach for Validation



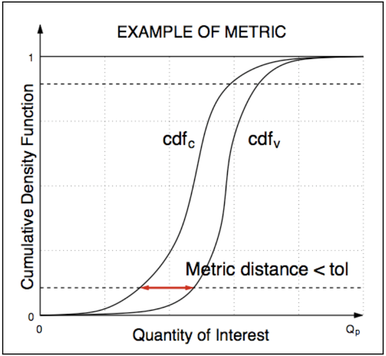
$$\mathcal{M}\left(\mathrm{O_{cal}}, \mathrm{D_{val}}\right) \leq \gamma_{\mathrm{tol}} \quad (?)$$

Proposed Validation Process (Babuška, Nobile, Tempone, 2009)



$$\mathcal{M}(Q_{cal}, Q_{val}) \leq \gamma_{tol} \quad (?)$$

Metric



Probability density functions:

$$p_C(Q) = p\big(Q\big(\mathbf{u}(p^C_{\text{post}}(\theta), s_p)\big)\big)$$

$$p_V(Q) = p\big(Q\big(\mathbf{u}(p^V_{\text{post}}(\theta), s_p)\big)\big)$$

Cumulative density functions:

$$\text{cdf}_C(Q) = \int_{-\infty}^{Q} p_C(Q)\, dQ$$

$$\text{cdf}_V(Q) = \int_{-\infty}^{Q} p_V(Q)\, dQ$$

Validation process requires detailed planning:

1. **Description of goals:** Describe background and goals of the predictions. Clearly define the quantity (or quantities) of interest.
2. **Modeling:** Write mathematical equations of selected model(s), list all parameters that are necessary to solve the problem, as well as assumptions and limitations of the model(s),
3. **Data collection:** Collect as many data as possible from literature or available sources (data should include, if available, the statistics).
4. **Sensitivity analysis:** Quantify the sensitivity of QoI with respect to parameters of the model. Rank parameters according to their influence.
5. **Calibration experiments:** Provide description of scenario (as precisely as possible), observables and statistics, prior and likelihood of the parameters to be calibrated.
6. **Validation experiments:** Provide same as above + clearly state assumption to be validated.

Morgan & Henrion's "Ten Commandements" (1990)*

In relation to quantitative risk and policy analysis

1. Do your homework with literature, experts and users.
2. Let the problem drive the analysis.
3. Make the analysis as simple as possible, but no simpler.
4. Identify all significant assumptions.
5. Be explicit about decision criteria and policy strategies.
6. Be explicit about uncertainties.
7. Perform systematic sensitivity and uncertainty analysis.
8. Iteratively refine the problem statement and the analysis.
9. Document clearly and completely.
10. Expose to peer review.

* Extracted from D. Vose, "Risk Analysis: A Quantitative Guide" (2008)

A systematic approach to the planning and implementation of experiments (Chapter 1 - Section 2)

In Wu & Hamada "Experiments, Analysis, and Optimization" (2009)

1. State objective.
2. Choose response.
3. Choose factors and levels.
4. Choose experimental plan.
5. Perform the experiment.
6. Analyze the data.
7. Draw conclusions and make recommendations:

   ... the conclusions should refer back to the stated objectives of the experiment. A confirmation experiment is worthwhile for example, to confirm the recommended settings. Recommendations for further experimentation in a follow-up experiment may also be given. For example, a follow-up experiment is needed if two models explain the experimental data equally well and one must be chosen for optimization.

Planning

- Planning is a cumbersome and time-consuming process.
- Planning of validation processes involves many choices that eventually need to be carefully checked.

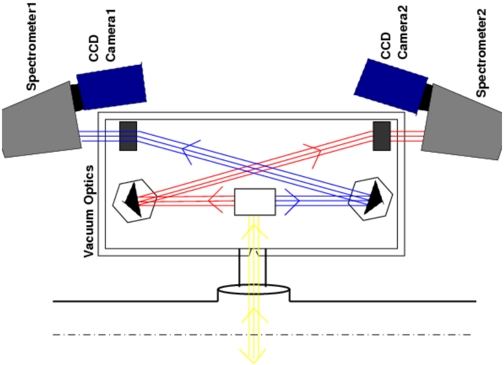
Choices are made about:

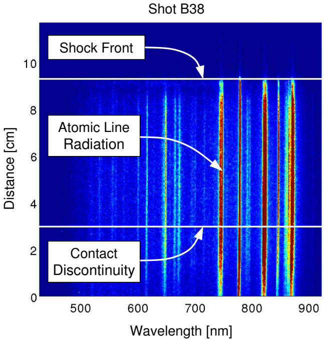
- Physical models
- Quantities of interest and surrogate quantities of interest
- Experiments for calibration and validation purposes
- Data sets to be used in calibration and validation
- Prior pdf and likelihood function
- Probabilistic models . . .

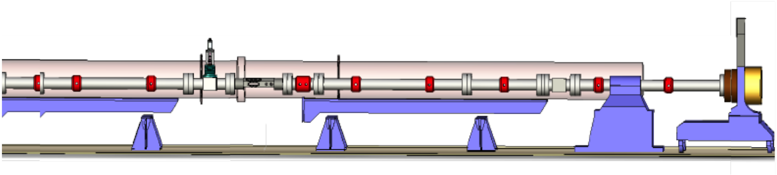
Our preliminary experiences with validation has revealed that many "sanity checks" need to be added within the proposed validation process.

Our objective is to develop a suite of tools to systematically verify the correctness of each stage of the validation process.

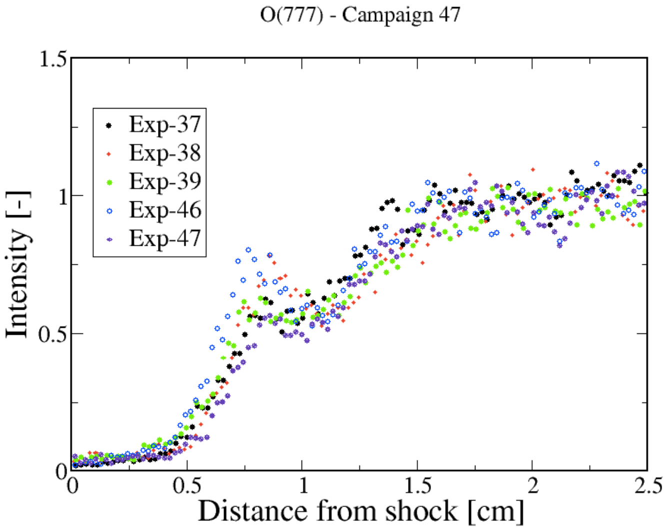
Examples: EAST (Shock-Tube) Experiments



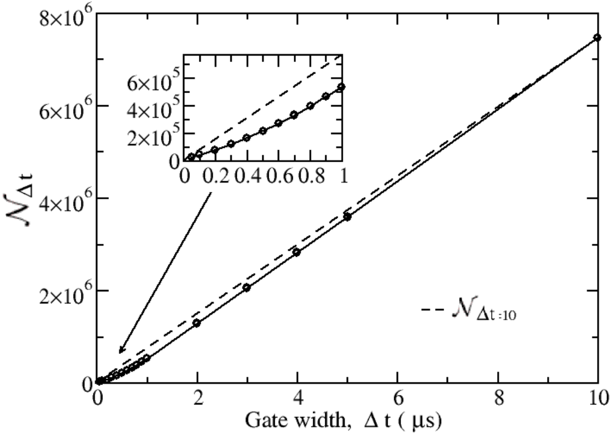




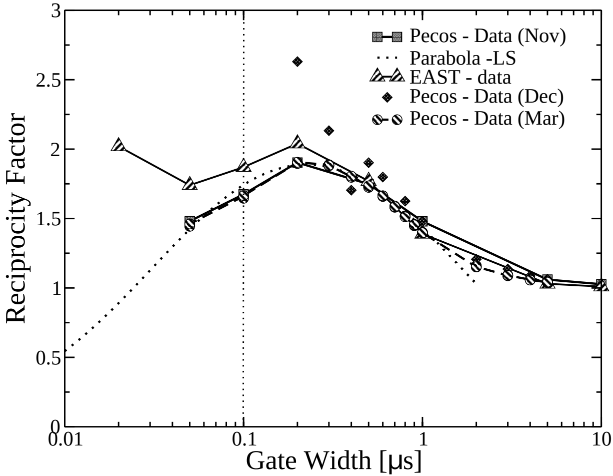
Data for Thermal and Chemical Non-equilibrium Models



Data reduction model for ICCD Camera

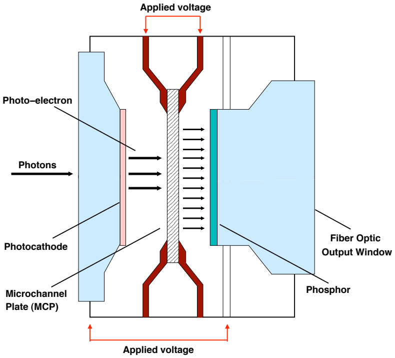


Data reduction model for ICCD Camera



The (non)-reciprocity factor quantifies the deviation w.r.t. the linear regime.

Data reduction model for ICCD Camera

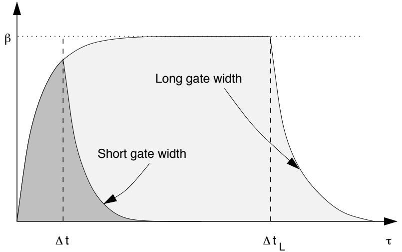


The opening/closing of the camera involves complex electronics phenomena. In shock-tube experiments at high speed, opening/closing of camera has to be done on the order of one microsecond. The major issue in this study was to identify whether the camera was being used in its linear or nonlinear regime for proper estimation of the intensity.

Validation Planning

Proposed physical models and corresponding model parameters.

[Based on RC circuits and "expert" opinion]



	α_1	α_2	β	δ	ν	Photon counts $\mathcal{N}_{\Delta t}$
M_1	✗	✗	✓	✗	✗	$\beta\Delta t$
M_2	✓	✓	✓	✗	✗	$\beta\Delta t - \Lambda(\Delta t, \alpha_1, \alpha_2, \beta)$
M_3	✓	✓	✓	✓	✗	$\beta(\Delta t + \delta) - \Lambda(\Delta t + \delta, \alpha_1, \alpha_2, \beta)$
M_4	✓	✓	✓	✗	✓	$(\beta + \nu)\Delta t - \Lambda(\Delta t, \alpha_1, \alpha_2\beta)$
M_5	✓	✓	✓	✓	✓	$(\beta + \nu)(\Delta t + \delta) - \Lambda(\Delta t + \delta, \alpha_1, \alpha_2\beta)$

Symbols ✓ or ✗ indicate that the parameter is or is not part of the model, respectively.

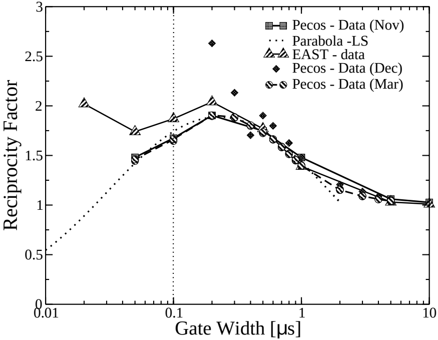
Validation Planning

QoI

- Reciprocity at $\Delta t = 0.1$ [μs]

Hypothesis to be validated

- Can the model(s) be predictive at low gate widths?



Calibration/Validation data

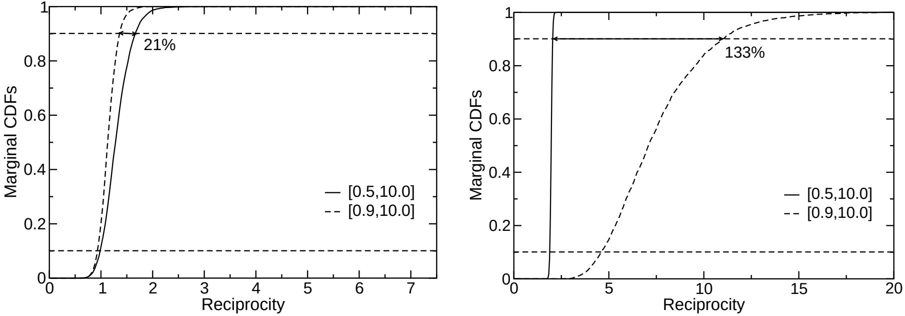
- Calibration data: in range 0.9 – 10.0 [μs]
- Validation data: in range 0.5 – 0.8 [μs]

Calibration

- Based on Bayesian inference.
- Uniform priors.
- Uncertainties in data and modeling error are combined.

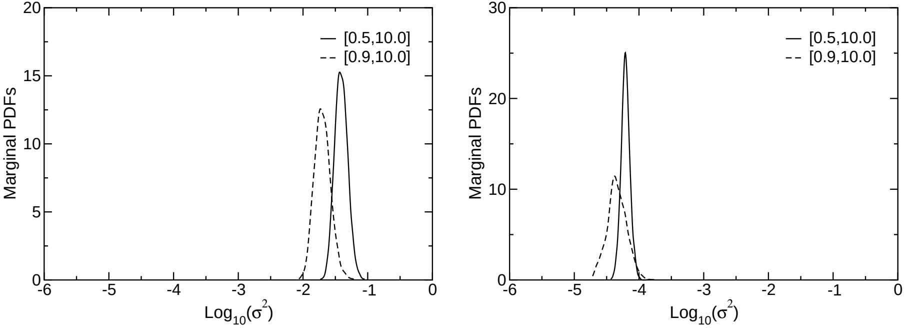
Results

CDF of QoI for model M1 (left) and model M5 (right):



Analysis of calibrated variance

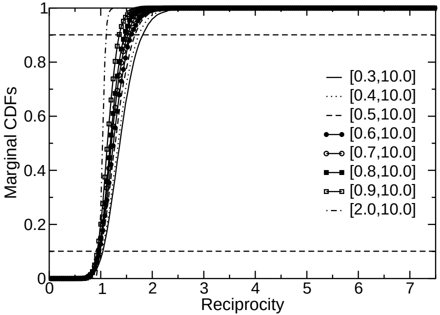
PDF of calibrated variance σ for model M1 (left) and model M5 (right):

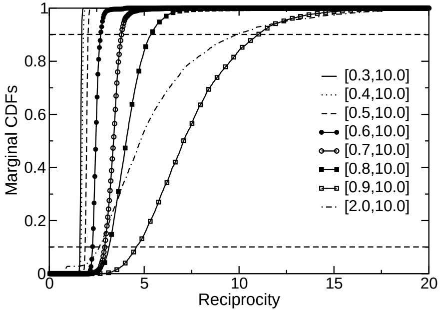


The validation process presupposes that the models can accurately predict observable data.

Convergence of calibration process with respect to number of data points

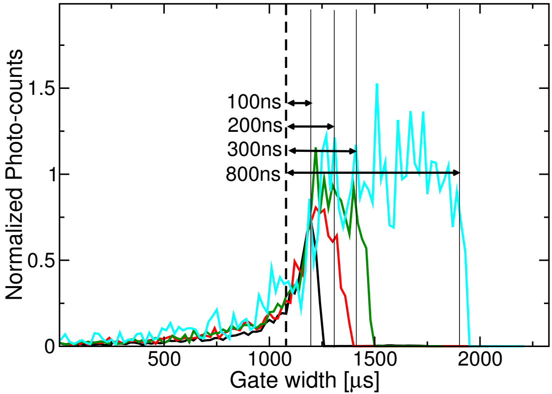
CDF of QoI for model M1 (left) and model M5 (right) for different data sets:





Models are rejected . . . and what?

- Acquire more data?
- Improve the models?



[From Aaron Brandis, NASA, September 2011]

Model Selection

Fully-developed incompressible channel flow:

Mean flow equations: $\boldsymbol{u} = \boldsymbol{U} + \boldsymbol{u}'$

$$\begin{cases} \nabla \cdot \left(\nu \nabla \boldsymbol{U} - \overline{\boldsymbol{u}_i' \boldsymbol{u}_j'} \right) = \rho^{-1} \nabla P \\ \nabla \cdot \boldsymbol{U} = 0 \end{cases}$$

Eddy-viscosity assumption:

$$\overline{\boldsymbol{u}_i' \boldsymbol{u}_j'} = -\nu_T \left(U_{i,j} + U_{j,i} \right)$$

Channel equations:

Assuming homogeneous turbulence in x, i.e. $U = U(y)$,

$$\partial_y \left((\nu + \nu_T) \partial_y U \right) = 1, \quad y \in (0, H)$$

Spalart-Allmaras (SA) model

Eddy viscosity is given by:

$$\nu_T = \tilde{\nu} f_{v1}, \qquad f_{v1} = \chi^3/(\chi^3 + {c_{v1}}^3), \qquad \chi = \tilde{\nu}/\nu$$

where $\tilde{\nu}$ is governed by the transport equation

$$\begin{aligned}\frac{D\tilde{\nu}}{Dt} &= \mathcal{P}_{\tilde{\nu}}(\kappa, c_{b1}) - \varepsilon_{\tilde{\nu}}(\kappa, c_{b1}, \sigma_{\mathsf{SA}}, c_{w2}) \\ &\quad + \frac{1}{\sigma_{\mathsf{SA}}}\left[\frac{\partial}{\partial x_j}\left((\nu + \tilde{\nu})\frac{\partial \tilde{\nu}}{\partial x_j}\right) + c_{b2}\left(\frac{\partial \tilde{\nu}}{\partial x_j}\right)^2\right]\end{aligned}$$

with

- $P_{\tilde{\nu}}$ = production term
- $D_{\tilde{\nu}}$ = wall destruction term

Parameter Values			
κ	0.41	c_{b2}	0.622
c_{b1}	0.1355	c_{v1}	7.1
σ_{SA}	2/3	c_{w2}	0.3

[1] Allmaras, Johnson, and Spalart, 2012; Oliver and Darmofal, 2009

Calibration data:

- Data is obtained from direct numerical simulation (DNS) [1]
- Mean velocity measurements at $Re_\tau = 944$ and $Re_\tau = 2003$

Uncertainty models:

- Three multiplicative error models

$$\langle u \rangle^+ (z;\xi) = (1 + \boldsymbol{\epsilon}(z;\xi))U^+(z;\xi)$$

  - independent homogeneous covariance
  - correlated homogeneous covariance
  - correlated inhomogeneous covariance

- Reynolds stress model

$$\left\langle \boldsymbol{u}_i' \boldsymbol{u}_j' \right\rangle^+ (z;\xi) = T^+(z;\xi) - \boldsymbol{\epsilon}(z;\xi)$$

[1] Del Alamo et al., 2004; Hoyas and Jiménez, 2006

Bayesian inference

Bayes rule:

$$\boxed{p(\boldsymbol{\theta}|\boldsymbol{D}) = \frac{L(\boldsymbol{\theta}|\boldsymbol{D})\, p(\boldsymbol{\theta})}{p(\boldsymbol{D})}} \quad \text{where} \begin{cases} \boldsymbol{D} \in \mathbb{R}^n & = \text{Calibration data} \\ L(\boldsymbol{\theta}|\boldsymbol{D}) & = \text{Likelihood} \\ p(\boldsymbol{\theta}) & = \text{Prior} \\ p(\boldsymbol{\theta}|\boldsymbol{D}) & = \text{Posterior} \end{cases}$$

Model selection:

- Set of models $\mathcal{M} = \{M_1, M_2, \ldots, M_n\}$
- Likelihood = $p(\boldsymbol{D}|M_i, \mathcal{M}) = \int_\theta p(\boldsymbol{D}|\boldsymbol{\theta}, M_i, \mathcal{M}) p(\boldsymbol{\theta}|M_i, \mathcal{M})\, d\boldsymbol{\theta}$
- Posterior plausibility = $p(M_i|\boldsymbol{D}, \mathcal{M})$

$$\boxed{p(M_i|\boldsymbol{D}, \mathcal{M}) \propto p(\boldsymbol{D}|M_i, \mathcal{M})\; p(M_i|\mathcal{M})}$$

- Evidence = $p(\boldsymbol{D})$

[1] QUESO (developed at ICES, UT Austin)

Numerical Results: Model selection

Model evidence ($\log(E)$):

	Surrogate	Full model
Independent homogeneous	-1.457	8.862
Correlated homogeneous	1.963	8.045
Correlated inhomogeneous	164.9	164.0
Reynolds stress	164.8	169.0

Relative runtimes (in seconds):

	Surrogate	Full model
Independent homogeneous	130	1720
Correlated homogeneous	162	1906
Correlated inhomogeneous	151	1735
Reynolds stress	147	1743
Cumulative	590	7104

Concluding remarks

1. Model validation is a complex, time-consuming, and CPU intensive process.
    - Model is never validated. It is at best not invalidated.
    - Validation should be performed on a prediction scenario with respect to given QoI's.
    - UQ should be included for comparison of data and computer outputs.
2. Validation planning requires insight and creativity.
    - Documentation
    - Data selection and analysis, etc.
3. Verification tools are needed to test correctness of processes.
    - Manufactured data to test calibration process
    - Sensitivity analysis to partially test the quality of the data
    - Evidence/plausibility to select best model among class of models
    - Tools to test selection of calibration and validation data sets
    - Tools to test various probabilistic models: prior pdf, likelihood
    - Experimental Design to select most informative experimental data